



chain nodes :

25 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

7-25 10-26 12-17

ring bonds :

1-2 1-6 1-10 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14 15-16
15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

7-25 10-26 12-17 15-16 15-20 16-17 17-18 18-19 19-20

normalized bonds :

1-2 1-6 1-10 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

G1:C,O,S

G2:Cl,Br,F,I,CH3,CH2,Et,CF2,OH,MeO,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 25:CLASS
26:CLASS